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Earlier self-consistent pseudopotential calculations of hetero- junction band lineups were refined. A rational electrostatic potential matching scheme was developed, involving the mean inter- stitial potential of the two semiconductors, shifted by a dipole contribution calculable from electronegativity data. A model for small crystallographic anisotropies is described.		

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## 1.) Introduction

This is the Final Report to ARO Grant # DAAG29-77-G-0017, "Theory of Heterojunction Discontinuities", for the period 1 November 1976 - 31 December 1977. The Principal Investigator was Dr. Herbert Kroemer, Professor of Electrical Engineering at the University of California at Santa Barbara (UCSB). The grant was a follow-up to an earlier grant (# DAHCO4-74-G-0114) to the University of Colorado, with the same Principal Investigator. A Final Report on the predecessor grant was issued in December 1976; the present report covers the follow-up grant only.

## 2.) The Problem

The problem studied was the theoretical understanding of the energy band lineup at semiconductor heterojunctions and the development of theoretical means to predict that lineup for new and as yet untried heterojunction pairs.

Heterojunctions are junctions between different semiconductors, such as GaAs and AlAs. They are increasingly being employed in advanced semiconductor devices, and the performance of the devices depends on the relative lineup of the energy bands at the junctions. Prior to the work under the present grant and its predecessor, the only rule for the prediction of the lineup was the electron affinity rule. It is theoretically ill-founded, and in practice hard to apply, because it requires empirical surface property data on high-quality crystals. Even where such data are available, the predictions made from them often do not agree with the results obtained on actual heterojunctions --once the latter have been prepared, often at great technological expense.

What was desired was a better theoretical understanding of why the heterojunctions line up the way they do, on a level that would make it possible to predict the lineup, with a minimum of technological investment, and thus to aid in making decisions as to whether or not the odds are favorable to make

it worthwhile to embark on the possibly very expensive technology to build a particular new device. We succeeded in developing theoretical techniques that have such a predictive capability.

Under the predecessor grant this work had reached the following stage.

A self-consistent pseudopotential method was developed that attempted to account for the known ionic core potential as realistically as possible before applying a repulsive pseudocore to the overall potential. By matching the calculated energy band structure of each semiconductor to the observed band structure, it was possible to determine the electrostatic potential outside the cores that goes hand-in-hand with this band structure. This permits expressing the band structure relative to a suitably chosen reference point on the electrostatic potential, a key step in determining heterojunction lineups. Such a reference potential should be chosen as far away from the ionic cores as possible. Two kinds of points suggested themselves: the halfway point along the interatomic bonds, and the points in the centers of the large interstitial sites. There are two kinds of interstitial sites in the compounds of interest, suggesting the average of the two interstitial potentials as a reference potential. When we made the ad hoc assumption that the latter reference potential be continuous across the heterojunction, we obtained lineups that agreed surprisingly well with observed lineups, much better than for other choices of the reference potential. However, the choice seemed to lack a good physical foundation. The best justification we could give it was a muffin-tin potential analogy that was not very satisfactory. Our first objective for the follow-up grant was to come up with a more rational electrostatic potential matching scheme.

### 3.) Results

We discovered early in the present grant that the mean interstitial potential is the potential at infinity if one treats the semiconductor as an assembly of spherical ions



bounded only by non-polar surfaces, and that it is therefore indeed the natural reference potential. Effective ionic charges for various semiconductors were determined and were found to correlate strongly with the difference in Phillips electronegativities between the constituent atoms of the semiconductor [1]. If one allocates one-quarter of each ionic charge to a charge transfer along each bond one can associate a charge transfer with each bond. If one applies this charge transfer to the bonds crossing the interface one obtains an estimate for an interface dipole by which the reference potentials on the two sides are shifted relative to each other [2].

Towards the end of the grant we modified the spherical ion model by assuming that there are actually charges located along the bonds. This leads to small corrections in the lineups, and to a small orientation-dependence of the heterojunction discontinuity. The correction is zero for (110) planes, has opposite values for (111)A and (111)B planes. The values for the two (100) planes are the same in this model as for the corresponding (111) planes. Numerical values can not be estimated at this point because of the absence of accurate values for the magnitude and location of the bond charges. This last work has not been published yet; a preprint is attached as Appendix.

During the last three months of the grant we briefly considered interface reconstruction effects and effects of grading, as in LPE junctions. No corrections of any significance were found.

#### 4.) Publications

- [1] W.R. Frensley and H. Kroemer, "Interstitial potential differences, electronegativity differences, and effective ionic charges in zinc-blende-type semiconductors," Appl. Phys. Lett. 31, 48(1977).
- [2] W.R. Frensley and H. Kroemer, "Theory of the energy-band lineup at an abrupt semiconductor heterojunction," Phys. Rev. B 16, 2642(1977).

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- [3] W.R. Frensley, "A theoretical study of the orientation dependence of heterojunction energy band lineups," to be published in the Proceedings of the 1978 Conference on the Physics of Compound Semiconductor Interfaces, J. Vac. Sci. Tech. -- preprint attached as Appendix.

5.) Participating Scientific Personnel

5.1) Principal Investigator: Dr. Herbert Kroemer, Professor of Electrical Engineering

5.2) Post-Doctoral Research Associate  
Dr. William R. Frensley.

5.3) Graduate Research Assistant  
Mr. Steve Wright, Graduate Student in Electrical Engineering.

No advanced degrees were earned under this follow-up grant.

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## APPENDIX

### A THEORETICAL STUDY OF THE ORIENTATION DEPENDENCE OF HETEROJUNCTION ENERGY BAND LINEUPS\*

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#### ABSTRACT

The orientation dependence of the energy band discontinuities at an abrupt semiconductor heterojunction is studied by modeling the microscopic charge distribution near the heterojunction. The model includes both ionic and bond charges, and assumes that each chemical bond contributes independently to the total charge distribution. The energy band lineups are derived by calculating the interface dipole. The results indicate that there should be no difference in the band lineups for heterojunctions on (100) and (111) faces of similar polarity. The lineup should be completely independent of orientation for heterojunctions which have an element common to both semiconductors, such as GaAs-AlAs. Any difference in band lineup between heterojunctions on nonpolar (110) planes and those on the (100) or (111) planes is related to deviations of the bond parameters from chemically systematic behavior, and thus is expected to be small.

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## I. Introduction

An important property of an abrupt semiconductor heterojunction is the change in energy band gap across the interface, which leads to discontinuities in the band-edge energies. The band gap change is distributed between the conduction and valence band discontinuities. The resulting band lineup is a property of the heterojunction, and it is an important consideration in the choice of heterojunction materials for a given device application.

We have previously proposed a method for theoretically predicting the band lineup at an abrupt heterojunction.<sup>1</sup> We divided the lineup problem into two parts. The first part concerned the calculation of the electronic band structure of the bulk semiconductors, and the relation of the band structure to the electrostatic crystal potential. The second part concerned the lineup of the electrostatic potential across the heterojunction, which was calculated from a model of the microscopic charge distribution near the interface. In the present work, we will investigate a more realistic model of the charge distribution, and emphasize the differences in band lineup which might occur between heterojunctions of similar composition, but which are fabricated on different crystallographic planes. Note that, within the above division of the problem, any orientation dependence must be due to differences in the charge distribution, not the bulk band structure.

## II. Independent Bond Model

In Reference 1 we took the valence charge distribution to be a linear superposition of spherical charges centered on the atomic sites. Such a model neglects an important feature of the true charge distribution in



tetrahedral semiconductors, which is the accumulation of charge between the atoms. Brill took this accumulation of charge into account in his X-ray analysis of diamond by introducing spherical bond charges midway between the carbon atoms,<sup>2</sup> and Phillips emphasized the structural role of the bond charge.<sup>3</sup> Walter and Cohen calculated the valence charge density of seven semiconductors using wavefunctions determined by the empirical pseudopotential method.<sup>4</sup> Their results indicate that the charge distribution can be well approximated by a superposition of spherical ionic and bond charges. As the ionicity of the crystal increases, the center of the bond charge moves toward the anion and the magnitude of the bond charge decreases. Of course, as the ionicity increases more of the valence charge is found in the vicinity of the anion.

Recently, calculational techniques have been developed which permit a self-consistent evaluation of the valence charge distribution in the vicinity of the surfaces<sup>5,6</sup> and interfaces.<sup>7,8</sup> The results of these calculations show some striking features. First, the perturbation in the charge distribution due to an interface extends over only a very short distance. Near a surface, the charge distribution assumes the bulk characteristics by the third atomic layer.<sup>5,6</sup> At a heterojunction the disturbance is even more short-ranged. Baraff, Appelbaum, and Hamann<sup>7</sup> have performed detailed calculations on a system consisting of three atomic layers of Ge on a semi-infinite GaAs crystal. They found that the charge distribution in the vicinity of the second Ge layer was indistinguishable from that of bulk Ge. Also, the bond charges between the Ge and Ga atoms had a magnitude intermediate between those of bulk Ge and GaAs. Moreover, they were able to determine the effective ionic charge associated with the interface bonds, and found that it was equal to one-half the corresponding value for bulk GaAs. All of this lends support to the notion that one can regard the

total valence charge distribution as a superposition of bond distributions, and that the chemical trends observed in the bulk semiconductors also hold for bonds at a heterojunction interface.

In this paper, we will conjecture that such behavior is a characteristic of all heterojunctions. Specifically, we will assume the following:

(i) the microscopic charge distribution is a linear superposition of individual charge distributions, each of which is associated with a single chemical bond, and (ii) those charge distributions are functions only of the chemical species being bonded. Thus, we assume that each bond contributes independently to the total valence charge distribution. We should emphasize that this is different from the approximations made in the linear-combination-of-atomic-orbitals (LCAO) theory of heterojunction lineups.<sup>9</sup> We do not assume that different bonds are not coupled by Hamiltonian matrix elements, but we do assume that the complete self-consistent solution to the interface charge density can be resolved into individual bonds.

The specific model of the microscopic charge distribution which we wish to investigate is described as follows. The charge distribution is assumed to be a linear superposition of spherical ionic and bond charges, with the ionic charges centered on the equilibrium atomic sites and the bond charges centered on some point along the line joining nearest neighbor atomic sites. The position of the center of the bond charge, measured from the anion, is denoted  $x$  and is expressed as a fraction of the bond length  $\sqrt{3} a/4$ , where  $a$  is the cubic lattice constant. Thus, the microscopic charge distribution may be completely described by the total charge contained in the ionic and bond charges, the width of their respective charge distributions, and the bond charge position  $x$ . If, however, we are only interested in evaluating

(9)

the electrostatic potential at a charge-free point (such as the interstitial point), we may, without loss of generality, take the width of the charge distributions to be zero (that is, to assume point charges). Therefore, we need only to consider the magnitude of the ionic and bond charges and the position of the bond charge.

Since the crystal must be electrically neutral and each bond contributes independently to the charge distribution, the charge distribution attributed to each bond must be neutral overall. This distribution consists of three charges (anion, cation, and bond charges), so the magnitudes of those charges must depend on only two parameters. The calculations will be simplified if we choose as parameters, the bond charge, denoted  $q_B$  and a transferred charge, denoted  $q_T$ . We assume that the bond charge is derived from both the anion and cation, with a charge  $xq_B$  coming from the cation and  $(1-x)q_B$  coming from the anion. The charge  $q_T$  is transferred from cation to anion. Thus the charge on the anion due to a single bond is

$$q_{\text{anion}} = q_T - (1-x) q_B, \quad (1)$$

and that the cation is

$$q_{\text{cation}} = -q_T - xq_B \quad (2)$$

as shown in Figure 1. The total charge on a given ion is simply the sum of the charges due to each of the four chemical bonds involving that ion.

We have previously<sup>1</sup> defined the dipole potential  $V_D$  as the difference between the mean interstitial potentials  $\bar{V}_i$  on either side of the heterojunction.

$$V_D = \bar{V}_i(1) - \bar{V}_i(2). \quad (3)$$



(10)

For the present calculations, it will be more convenient to consider the spatially averaged potential  $\bar{V}$  and its difference across the heterojunction

$$\Delta\bar{V} = \bar{V}(1) - \bar{V}(2) \quad (4)$$

The quantities  $\bar{V}_i$  and  $\bar{V}$  can be related, within the bulk semiconductor, by a Madelung-type calculation. We have previously described such a calculation for a spherical ion model.<sup>10</sup> To take the bond charges into account, we consider a lattice of charges  $q_B$  located at the bond charge sites and charges  $-2q_B$  located at the atomic sites. The potential at an interstitial point of this lattice can be expressed by

$$V(i) = \frac{\beta_i(x) q_B}{4\pi\epsilon_0 a} \quad (5)$$

where  $i = 1, 2$  denotes the two inequivalent interstices. The values of  $\beta$  are evaluated with the boundary condition that the spatially averaged potential equals zero. Therefore, we can relate  $\bar{V}_i$  and  $\bar{V}$  by

$$\bar{V}_i = \bar{V} + \frac{\beta^+(x) q_B}{4\pi\epsilon_0 a} \quad (6)$$

Also, the interstitial potential difference  $\Delta V_i$  is

$$\Delta V_i = \frac{8\alpha[q_T - (\frac{1}{2} - x)q_B] + 2\beta^-(x)q_B}{4\pi\epsilon_0 a} \quad (7)$$

where  $\alpha=0.2878$  for the zincblende structure.<sup>10</sup> In the above expressions

$$\beta^+ = \frac{1}{2}(\beta_1 + \beta_2) \quad (8a)$$

$$\beta^- = \frac{1}{2}(\beta_1 - \beta_2) \quad (8b)$$



The functions  $\beta^+(x)$  and  $\beta^-(x)$  are graphed in Figure 2.

We may now apply this model to the calculation of the interface dipole at a heterojunction. We consider an ideally abrupt heterojunction between compounds AB and CD. The parameters of the charge distribution depend only on the atomic species connected by each bond. For example,  $q_B(AB)$ ,  $q_T(AB)$ , and  $x(AB)$  are the parameters of the A-B bonds in the bulk crystal, while  $q_B(CB)$ ,  $q_T(CB)$ , and  $x(CB)$  describe the C-B bonds occurring at the interface. To evaluate the dipole, we average the charge distribution over the planes parallel to the interface. The dipole calculation then becomes a simple one dimensional electrostatic problem. Explicit calculations for heterojunctions on the (100), (111), and (110) planes give the following results. The dipoles, and therefore the band lineups, are equal for (100) and (111) junctions of similar polarity. If, for example, the B and C atomic planes are adjacent to the interface, the difference in mean potentials is given by

$$\begin{aligned} \Delta\bar{V}(111) = \frac{1}{2\epsilon_0 a} \{ & 2q_T(CB) - q_T(AB) - q_T(CD) \\ & + x(CD) [1-x(CD)]q_B(CD) - x(AB) [1-x(AB)]q_B(AB) \} \end{aligned} \quad (9)$$

The first three terms in the above expression represent the transfer of charge which actually gives rise to the dipole while the last two terms are due to the effect of the bond charge on the mean potential in the bulk. If the heterojunction is of the opposite polarity, that is, if the A and D atoms are bonded across the interface, the mean potential shift is

(12)

$$\begin{aligned} \Delta \bar{V}(\bar{1}\bar{1}\bar{1}) = & \frac{1}{2\epsilon_0 a} \{-2 q_T(AD) + q_T(AB) + q_T(CD) \\ & + x(CD) [1-x(CD)] q_B(CD) - x(AB) [1-x(AB)] q_B(AB)\}. \end{aligned} \quad (10)$$

For a heterojunction on a nonpolar (110) plane,  $\Delta \bar{V}$  is given by

$$\begin{aligned} \Delta \bar{V}(110) = & \frac{1}{2\epsilon_0 a} \{q_T(CB) - q_T(AD) + x(CD) [1-x(CD)] q_B(CD) \\ & - x(AB) [1-x(AB)] q_B(AB)\} \end{aligned} \quad (11)$$

If we take the differences between the above expressions, we find

$$\begin{aligned} \Delta \bar{V}(111) - \Delta \bar{V}(110) = & \Delta \bar{V}(110) - \Delta \bar{V}(\bar{1}\bar{1}\bar{1}) = \\ & \frac{1}{2\epsilon_0 a} \{q_T(AD) + q_T(CB) - q_T(AB) - q_T(CD)\} \end{aligned} \quad (12)$$

Therefore, the dipole for a (110) heterojunction is equal to the mean of the dipoles for (111) and ( $\bar{1}\bar{1}\bar{1}$ ) heterojunctions.

An examination of equation (12) shows that if  $q_T$  can be written as a difference between ionic parameters, there will be no orientation dependence of the band lineups. This is similar to the results derived in Reference 1. Also, for a heterojunction between compounds which share a common element, such as GaAs - AlAs, there will be no orientation dependence. In such a heterojunction on a polar orientation, the position of the interface plane is ambiguous, so there is no distinction between (100) and ( $\bar{1}\bar{0}\bar{0}$ ) heterojunctions, for example.

The above expressions can be applied to the prediction of heterojunction lineups given the parameters of the charge distribution. Unfortunately,

(13)

when we included the bond charges in the valence charge model, we also included the uncertainty in the magnitude of those charges, and the other model parameters are rather sensitive to such uncertainties. A natural way to determine the model parameters would be the following. First the bond charge location  $x$  and magnitude  $q_B$  should be determined for the bulk semiconductors from the valence charge distribution calculations. The transferred charge  $q_T$  could then be calculated from the interstitial potential difference  $\Delta V_i$  by solving equation (7). Chemical trends in the parameters so determined, such as those discussed in Reference 10, could then be used to estimate the parameters of bonds not occurring in the bulk semiconductors (such as Ge-Ga). The sensitivity of this procedure arises from the solution of equation (7), where small changes in  $q_B$  produce larger changes in the calculated values of  $q_T$ .

In spite of the difficulties we can make some general statements about the effect of the bond charges on the energy band lineup. Only the bond charges of the bulk semiconductor appear in equations (8) and (9)-(11). We may interpret those terms containing the bond charges raising the bulk energy bands by an amount

$$\Delta E_{BC} = \frac{\beta^+(x)q_B}{4\pi\epsilon a} + \frac{x(1-x)q_B}{2\epsilon_0 a} \quad (13)$$

If we use Walter and Cohen's estimates of  $q_B$  (Ge) = 0.146e and  $q_B$  (GaAs) = 0.080<sup>4</sup> along with the values  $x(\text{Ge}) = 0.50$  and  $x(\text{GaAs}) = 0.37$  from our calculations, we get  $\Delta E_{BC}(\text{Ge}) = 0.92$  eV and  $\Delta E_{BC}(\text{GaAs}) = 0.46$  eV. Therefore, including the bond charge can have a significant effect on the energy band

(14)

lineup. In general, since the magnitude of the bond charge decreases with increasing ionicity, we would expect the bond charge effects to raise the bands of the group IV semiconductors with respect to the III-V compounds and raise the III-V's with respect to the II-VI's.

### III. Discussion and Conclusions

We have presented a model of the microscopic charge distribution near a semiconductor heterojunction which includes the effects of bond charges. The parameters of the model are not yet sufficiently well determined that it may be used to predict actual heterojunction band lineups. However, the model does provide a basis for comparing the energy band lineups of heterojunctions of the same chemical composition but fabricated on different crystallographic orientations. We find that heterojunctions on polar (100) and (111) planes of the same polarity should have identical band lineups. Nonpolar (110) heterojunctions should have a band lineup equal to the mean of the (111) and ( $\bar{1}\bar{1}\bar{1}$ ) lineups. Junctions involving a common ion, such as GaAs-AlAs, should exhibit no orientation dependence.

A very interesting feature of the model is the form of the expression for the difference between interface dipoles on different orientations (equation (2)). This expression demonstrates the role of systematic chemical behavior in heterojunction lineups. For example, if we could write

$$q_T(AB) = X(A) - X(B), \quad (14)$$

where  $X$  is a property of the atomic species only, then we would have

$$a_T(AD) + q_T(CB) - q_T(AB) - q_T(CD) = 0 \quad (15)$$



(15)

Thus, equation (12) is an expression of the deviation from chemically systematic behavior of the transferred charge  $q_T$ . We may therefore expect the orientation dependence of the band lineup to be small.

The only experimental evidence of an orientation dependence are the old Ge-GaAs data of Fang and Howard.<sup>11</sup> They found a difference of about 0.2 eV in the mean conduction band discontinuity between the different crystallographic orientations. However, the scatter in their data for any given orientation was of about the same magnitude. It is interesting to note that if equation (15) were violated to the extent of 0.01 electron (an estimate based on the results in Reference 10), the heterojunction lineups of the different orientations would differ by about 0.15 eV. However, Fang and Howard found the conduction band discontinuity of both the (111) and  $(\bar{1}\bar{1}\bar{1})$  heterojunctions to be larger than that for the (110) junction, in contrast to our prediction that the (110) discontinuity should lie between the discontinuities for the polar orientations.

Finally, we should note that  $q_T$  is a measure of the net dipole moment of the charge distribution associated with a band. Such a quantity can be defined for any charge distribution, not just for the model studied here. We therefore believe that the result given by equation (12), expressing the relation between the band lineup and the systematic behavior of the bond properties, would hold for any model in which the bonds contribute independently to the charge distribution.

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## Footnotes

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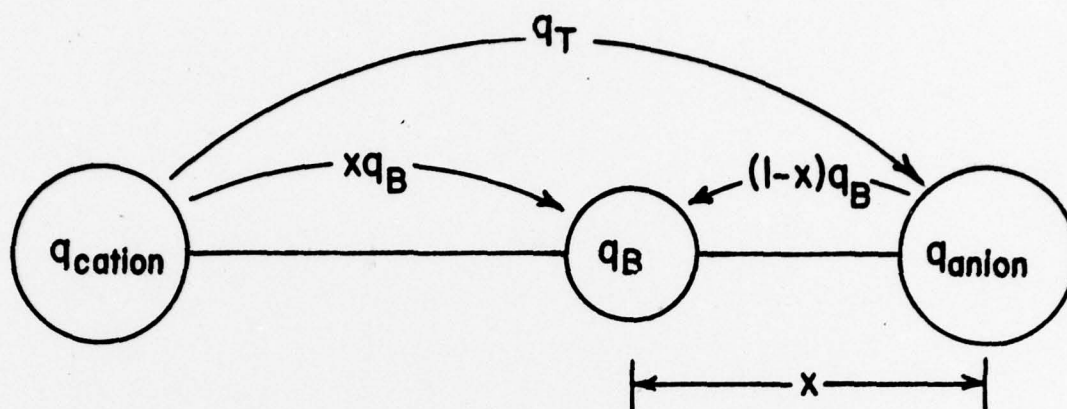
Figure Captions

Figure 1. A schematic representation of the assumed form of the charge distribution associated with each chemical bond.

Figure 2. The Madelung-type functions  $\beta^+$  and  $\beta^-$ , which describe the effect of the bond charges on the interstitial potentials, as a function of the bond charge position  $x$ .



(19)



(20)

